* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:13:23 ON 07 SEP 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:13:32 ON 07 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 SEP 2004 HIGHEST RN 740796-45-6
DICTIONARY FILE UPDATES: 6 SEP 2004 HIGHEST RN 740796-45-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
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L1 STRUCTURE UPLOADED

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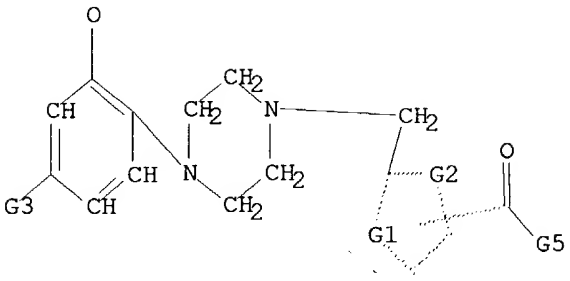
L2 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 S,N

G2 C,O,N

G3 C,H,O

G4 O,X

G5 H,O

Structure attributes must be viewed using STN Express query preparation.

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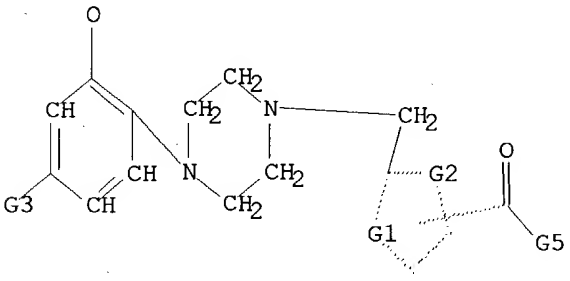
L2 HAS NO ANSWERS
L2 STR



G1 S,N

G2 C,O,N

G3 C,H,O

G4 O,X

G5 H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 16:14:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1641 TO ITERATE

100.0% PROCESSED 1641 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L3 6 SEA SSS FUL L1

=> s l2 sss full

FULL SEARCH INITIATED 16:15:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1641 TO ITERATE

100.0% PROCESSED 1641 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L4 6 SEA SSS FUL L2

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	311.26	311.47

FILE 'CAPLUS' ENTERED AT 16:15:06 ON 07 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 7 Sep 2004 VOL 141 ISS 11
FILE LAST UPDATED: 6 Sep 2004 (20040906/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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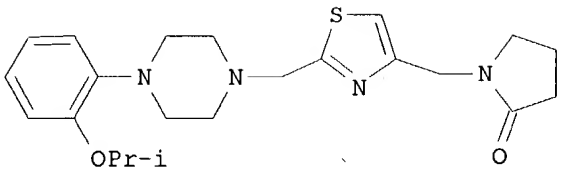
L5 3 L3

=> d l5 1-3 ibib abs hitstr

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:585086 CAPLUS
DOCUMENT NUMBER: 138:89769
TITLE: Arylpiperazine substituted heterocycles as Selective αla adrenergic antagonists
AUTHOR(S): Khatuya, Haripada; Hutchings, Richard H.; Kuo, Gee-Hong; Pulito, Virginia L.; Jolliffe, Linda K.; Li, Xiaobing; Murray, William V.
CORPORATE SOURCE: Drug Discovery Research, Johnson & Johnson Pharmaceutical Research and Development LLC, Raritan, NJ, 08869, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(17), 2443-2446
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89769
GI



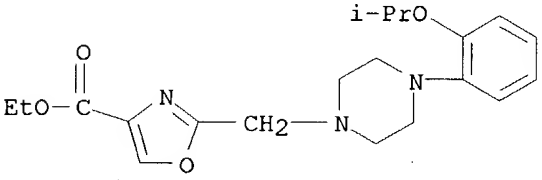
I

AB Antagonists of the α1-adrenergic receptors (α1-ARs) are useful for the treatment of benign prostatic hyperplasia. A series of potent and subtype-selective α1a-AR antagonists has been synthesized, e.g. I, displaying in vitro binding affinity in the low the nanomolar range.

IT **483987-66-2P 483987-69-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylpiperazine substituted heterocycles as selective α1a adrenergic antagonists)

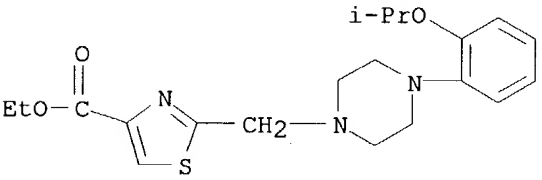
RN 483987-66-2 CAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 483987-69-5 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:543677 CAPLUS

DOCUMENT NUMBER: 138:39156

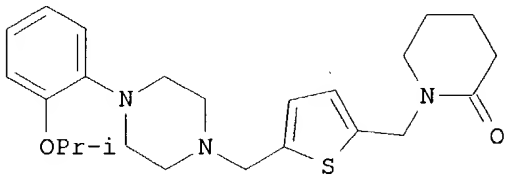
TITLE: Novel thiophene derivatives for the treatment of benign prostatic hyperplasia

AUTHOR(S): Khatuya, Haripada; Pulito, Virginia L.; Jolliffe, Linda K.; Li, Xiaobing; Murray, William V.

CORPORATE SOURCE: Drug Discovery Research, Johnson & Johnson Pharmaceutical Research and Development LLC, Raritan, NJ, 08869, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),

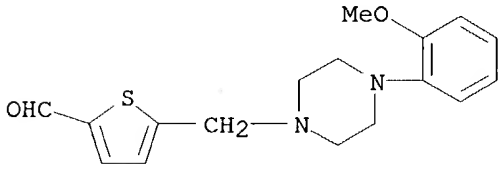
12(16), 2145-2148
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:39156
GI



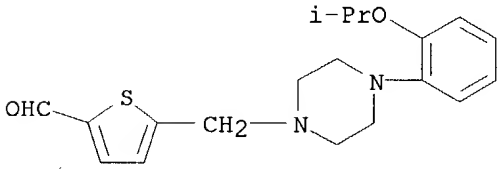
I

AB The syntheses and biol. activities of a novel series of 2,4- and 2,5-disubstituted thiophenes, e.g. I, are reported. These analogs have shown excellent affinity and selectivity against α1-adrenoreceptor subtypes.

IT **223254-07-7P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(novel thiophene derivs. for the treatment of benign prostatic hyperplasia)
RN 223254-07-7 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



IT **478811-76-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel thiophene derivs. for the treatment of benign prostatic hyperplasia)
RN 478811-76-6 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:271334 CAPLUS
DOCUMENT NUMBER: 130:296696
TITLE: Preparation of arylpiperazines for the treatment of benign prostatic hyperplasia.
INVENTOR(S): Hutchings, Richard H.; Khatuya, Haripada; Kuo, Gee-Hong; Li, Xiaobing; Murray, William V.; Prouty, Catherine
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9919299	A1	19990422	WO 1998-US21470		19981009
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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AU 9910783	A1	19990503	AU 1999-10783		19981009
EP 1025085	A1	20000809	EP 1998-953393		19981009
EP 1025085	B1	20030326			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
JP 2001519413	T2	20011023	JP 2000-515872		19981009
US 6384035	B1	20020507	US 1998-169571		19981009
EP 1273572	A1	20030108	EP 2002-78537		19981009
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
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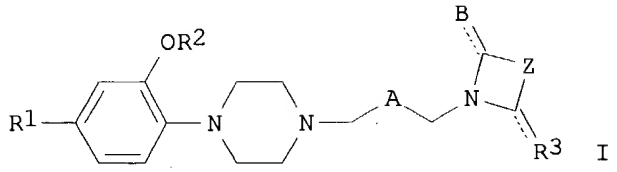
ES 2195410	T3	20031201	ES 1998-953393		19981009
HK 1026701	A1	20031121	HK 2000-105885		20000919
US 2002165219	A1	20021107	US 2001-994153		20011126
PRIORITY APPLN. INFO.:			US 1997-61618P	P	19971009
			EP 1998-953393	A3	19981009
			US 1998-169571	A3	19981009
			WO 1998-US21470	W	19981009

OTHER SOURCE(S): MARPAT 130:296696
GI



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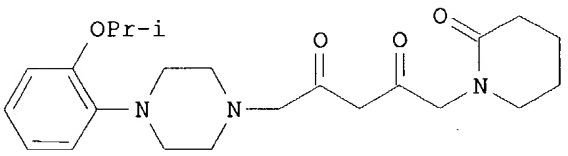


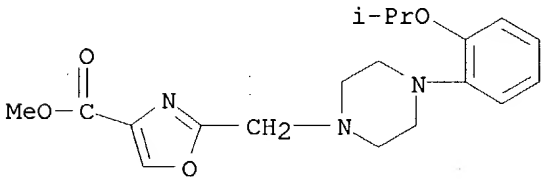
II

AB Title compds. [I; R1 = H, halo, alkoxy, OH, alkyl; R2 = (substituted) alkyl, Ph, phenylalkyl; R3 = H, alkoxycarbonyl, alkyl, hydroxyalkyl, CHO, Ac, amido, O; A = oxazolylidene, thienylene, isoxazolidene, COCH2CO, COCH2CHOH, COCH:CH, CHOHCH2CHOH, etc.; B = H, O; Z = (CH2)n, etc.; n = 1-5; dotted lines = double bonds when R3, B = O], were prepared Thus, chloroacetone was refluxed with 1-(2-isopropoxyphenyl)piperazine and K2CO3 for 1 day to give 1-(2-isopropoxyphenyl)-4-(2-oxopropyl)piperazine. The latter was stirred with 1-(ethoxycarbonylmethyl)-2-piperidone and NaH in THF to give title compound (II), which showed bound to adrenergic α1a, α1b, and α1c receptors with IC50 = 417 nM, >10000 nM, and 6043 nM, resp.

IT **223253-82-5P 223253-94-9P 223254-07-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylpiperazines for the treatment of benign prostatic hyperplasia)

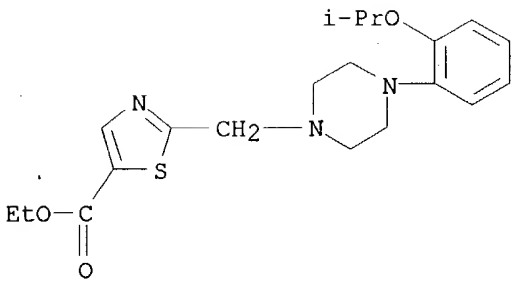
RN 223253-82-5 CAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

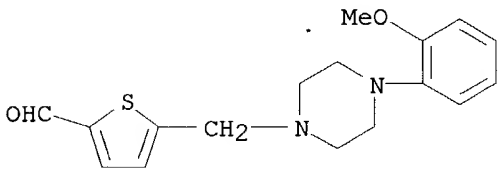


RN 223253-94-9 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 223254-07-7 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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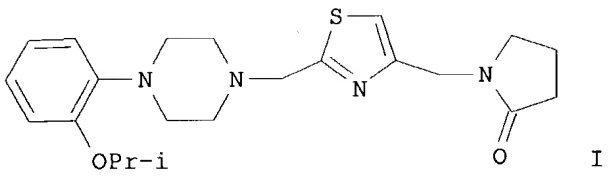
L6 3 L4

=> d l6 1-3 ibib abs hitstr

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:585086 CAPLUS
DOCUMENT NUMBER: 138:89769
TITLE: Arylpiperazine substituted heterocycles as Selective α1a adrenergic antagonists
AUTHOR(S): Khatuya, Haripada; Hutchings, Richard H.; Kuo, Gee-Hong; Pulito, Virginia L.; Jolliffe, Linda K.; Li, Xiaobing; Murray, William V.
CORPORATE SOURCE: Drug Discovery Research, Johnson & Johnson Pharmaceutical Research and Development LLC, Raritan, NJ, 08869, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(17), 2443-2446
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89769
GI



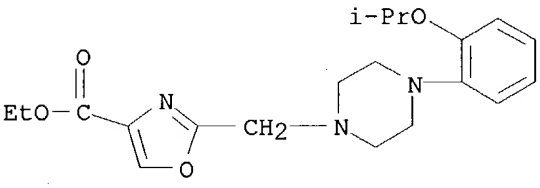
I

AB Antagonists of the α1-adrenergic receptors (α1-ARs) are useful for the treatment of benign prostatic hyperplasia. A series of potent and subtype-selective α1a-AR antagonists has been synthesized, e.g. I, displaying in vitro binding affinity in the low the nanomolar range.

IT **483987-66-2P 483987-69-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylpiperazine substituted heterocycles as selective α1a adrenergic antagonists)

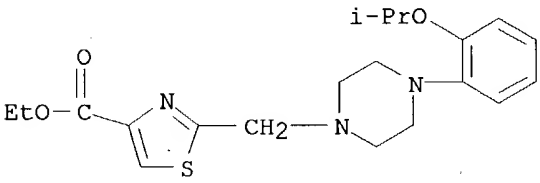
RN 483987-66-2 CAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 483987-69-5 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:543677 CAPLUS

DOCUMENT NUMBER: 138:39156

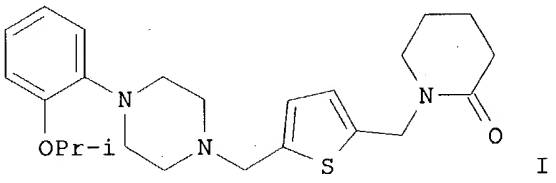
TITLE: Novel thiophene derivatives for the treatment of benign prostatic hyperplasia

AUTHOR(S): Khatuya, Haripada; Pulito, Virginia L.; Jolliffe, Linda K.; Li, Xiaobing; Murray, William V.

CORPORATE SOURCE: Drug Discovery Research, Johnson & Johnson Pharmaceutical Research and Development LLC, Raritan, NJ, 08869, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(16), 2145-2148
CODEN: BMCLE8; ISSN: 0960-894X

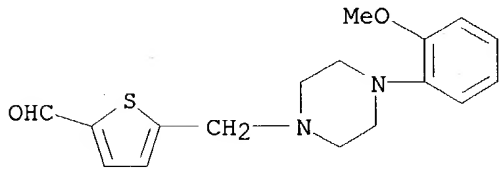
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:39156
GI



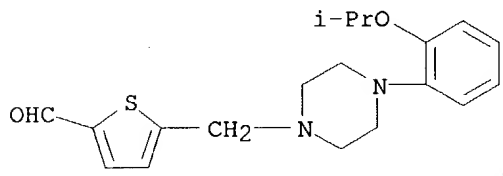
I

AB The syntheses and biol. activities of a novel series of 2,4- and 2,5-disubstituted thiophenes, e.g. I, are reported. These analogs have shown excellent affinity and selectivity against α1-adrenoreceptor subtypes.

IT **223254-07-7P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(novel thiophene derivs. for the treatment of benign prostatic hyperplasia)
RN 223254-07-7 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



IT **478811-76-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel thiophene derivs. for the treatment of benign prostatic hyperplasia)
RN 478811-76-6 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



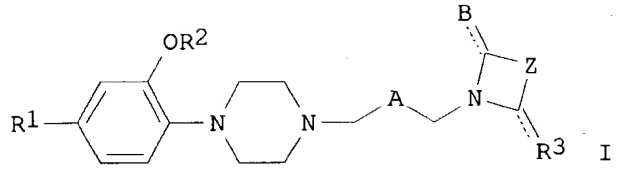
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:271334 CAPLUS
DOCUMENT NUMBER: 130:296696
TITLE: Preparation of arylpiperazines for the treatment of benign prostatic hyperplasia.
INVENTOR(S): Hutchings, Richard H.; Khatuya, Haripada; Kuo, Gee-Hong; Li, Xiaobing; Murray, William V.; Prouty, Catherine
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9919299	A1	19990422	WO 1998-US21470	19981009
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2305353	AA	19990422	CA 1998-2305353	19981009
AU 9910783	A1	19990503	AU 1999-10783	19981009
EP 1025085	A1	20000809	EP 1998-953393	19981009
EP 1025085	B1	20030326		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2001519413	T2	20011023	JP 2000-515872	19981009
US 6384035	B1	20020507	US 1998-169571	19981009
EP 1273572	A1	20030108	EP 2002-78537	19981009
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 235466	E	20030415	AT 1998-953393	19981009
ES 2195410	T3	20031201	ES 1998-953393	19981009
HK 1026701	A1	20031121	HK 2000-105885	20000919
US 2002165219	A1	20021107	US 2001-994153	20011126

PRIORITY APPLN. INFO.:		
US 1997-61618P	P	19971009
EP 1998-953393	A3	19981009
US 1998-169571	A3	19981009
WO 1998-US21470	W	19981009

OTHER SOURCE(S): MARPAT 130:296696
GI



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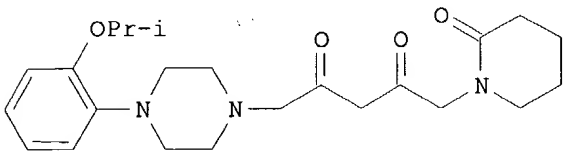


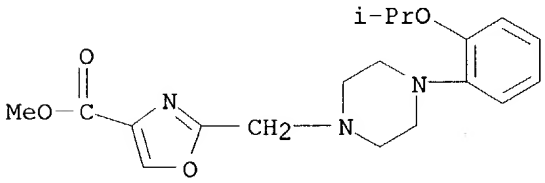
II

AB Title compds. [I; R1 = H, halo, alkoxy, OH, alkyl; R2 = (substituted) alkyl, Ph, phenylalkyl; R3 = H, alkoxycarbonyl, alkyl, hydroxyalkyl, CHO, Ac, amido, O; A = oxazolylidene, thienylene, isoxazolidene, COCH2CO, COCH2CHOH, COCH:CH, CHOHCH2CHOH, etc.; B = H, O; Z = (CH2)n, etc.; n = 1-5; dotted lines = double bonds when R3, B = O], were prepared Thus, chloroacetone was refluxed with 1-(2-isopropoxyphenyl)piperazine and K2CO3 for 1 day to give 1-(2-isopropoxyphenyl)-4-(2-oxopropyl)piperazine. The latter was stirred with 1-(ethoxycarbonylmethyl)-2-piperidone and NaH in THF to give title compound (II), which showed bound to adrenergic α1a, α1b, and α1c receptors with IC50 = 417 nM, >10000 nM, and 6043 nM, resp.

IT **223253-82-5P 223253-94-9P 223254-07-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylpiperazines for the treatment of benign prostatic hyperplasia)

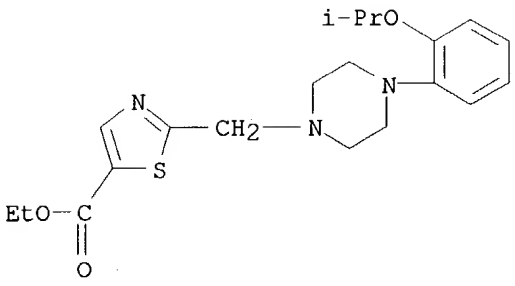
RN 223253-82-5 CAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

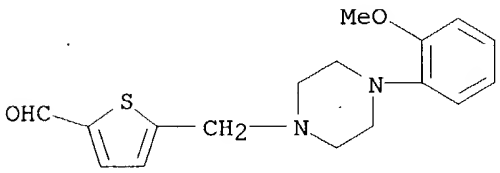


RN 223253-94-9 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[4-[2-(1-methylethoxy)phenyl]-1-piperazinyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 223254-07-7 CAPLUS
CN 2-Thiophenecarboxaldehyde, 5-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT